

Orizalyn

Inchi:	InChI=1S/C12H18N4O6S/c1-3-5-14(6-4-2)9-7-10(15(17)18)12(23(13,21)22)11(8-9)16(19)
InchiKey:	UQMCMYWIBUCJDH-UHFFFAOYSA-N
Formula:	C12H18N4O6S
SMILES:	CCCN(CCC)c1cc([N+](=O)[O-])c(S(N)(=O)=O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	346.36

Physical Properties

Property code	Value	Unit	Source
gf	-86.53	kJ/mol	Joback Method
hf	-462.44	kJ/mol	Joback Method
hfus	62.03	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	1.777		Crippen Method
mcvol	239.070	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	952.01	K	Joback Method
tc	1192.53	K	Joback Method
tf	730.49	K	Joback Method
vc	0.936	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.32	J/mol×K	952.01	Joback Method
cpg	744.75	J/mol×K	992.10	Joback Method
cpg	752.94	J/mol×K	1032.18	Joback Method
cpg	759.93	J/mol×K	1072.27	Joback Method
cpg	765.76	J/mol×K	1112.36	Joback Method
cpg	770.46	J/mol×K	1152.44	Joback Method
cpg	774.09	J/mol×K	1192.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566620&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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